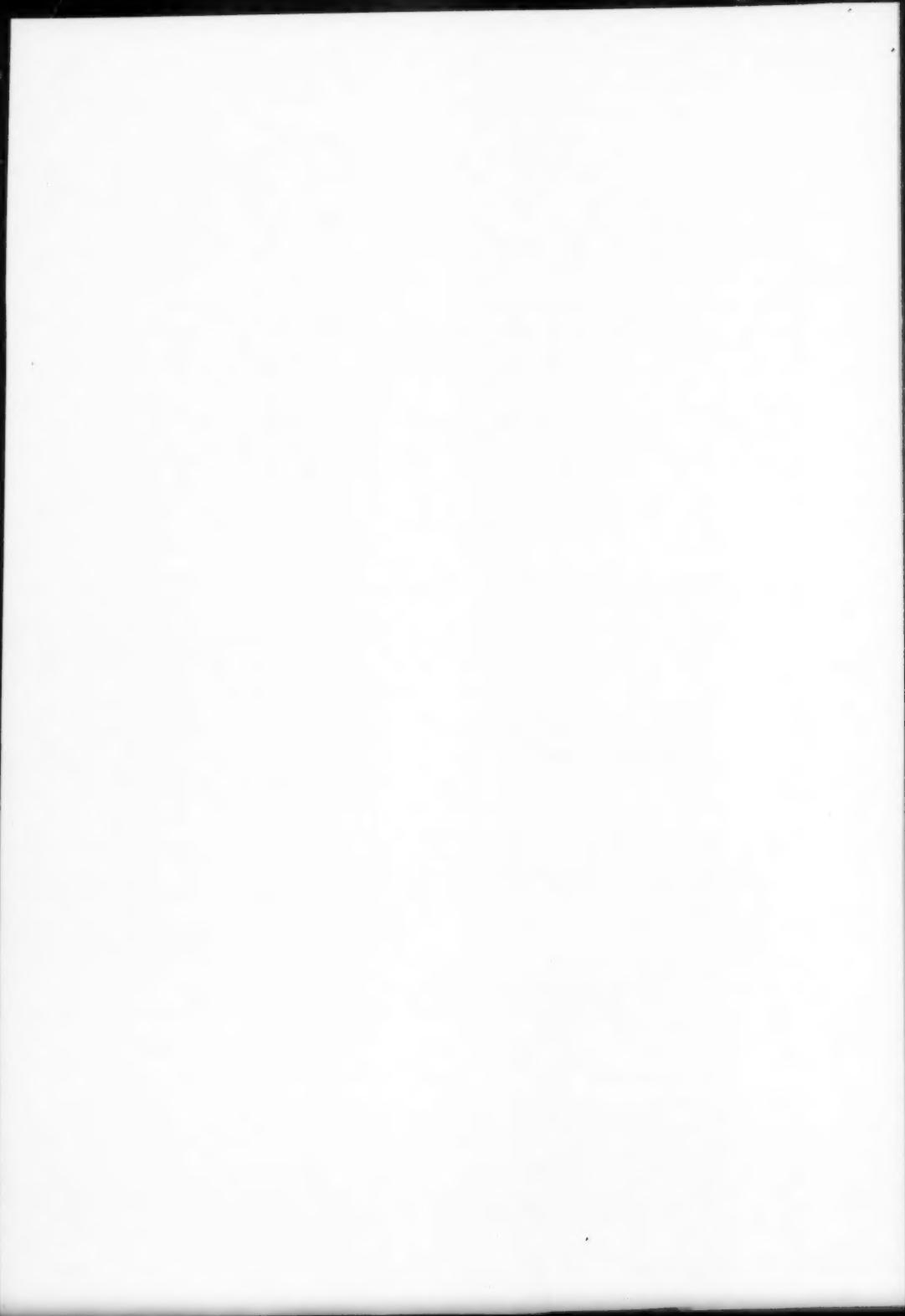


ACTA POLYTECHNICA SCANDINAVICA

ANNOTATED INDEX 1986

HELSINKI 1987



ACTA POLYTECHNICA SCANDINAVICA

Annotated Index 1986

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ABSTRACTS

CHEMICAL TECHNOLOGY AND METALLURGY SERIES

(formerly Chemistry including Metallurgy Series, ISSN 0001-6853)

Ch 168

UDC 517.93:66.095.2

Heiskanen, T., *Stability of Continuous Emulsion Polymerization of Vinyl Chloride, and Computer Simulation of Its Nonlinear Dynamic Behavior*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 168, Helsinki 1986, 60 pp. ISBN 951-666-223-4. ISSN 0781-2698.

Key words: Continuous emulsion polymerization, vinyl chloride, stability, nonlinear dynamics, computer simulation.

Dynamic moment equations were used to study the stability and dynamics of continuous emulsion polymerization of vinyl chloride. Stability was studied by numerically solving the eigenvalues of the linearized moment equations with several combinations of parameters. The linearized system was found to be stable or unstable depending on parameter values. It was found that the system could be stabilized by decreasing the residence time, increasing the emulsifier concentration, or decreasing the initiator concentration.

The dynamic behavior of the nonlinear moment equations were studied by numerically solving the nonlinear dynamic moment equations with different initial conditions, and assuming no external disturbances.

The system exhibited either decay of transients or limit cycles depending on the stability of the respective steady-state. The dynamic responses were shown both in phase-space and time domain.

Ch 169

UDC 66.063:532.529.2/3

Ogawa, K. and Kuroda, C., *Application of Swirling Jets to Mixing of Stratified Liquid Layers*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 169, Helsinki 1986, 28 pp. ISBN 951-666-224-2. ISSN 0781-2698.

Key words: Stratified liquid, swirling jet.

The swirling jet mixing which is adopted as simple and effective method for mixing of stratified two liquid layers is investigated on the basis of the experimental results about the mixing process in a swirling jet of a single fluid. The general Reynolds number Re and the Reynolds number of swirl $Re\theta$ are used as representative dimensionless quantities of operational conditions and it is made clear how to determine the adequate operational conditions for mixing of stratified two liquid layers. When the operational conditions are determined, the method for estimating the power consumption in the swirling jet equipment is shown by using the previous results about the decay process of swirling pipe flow.

Judin, V.-P., *Single Ion Activity Measurements in the System Hydrochloric Acid — Aluminum Chloride — Water by the Electromotive Force Method*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 170, Helsinki 1986, 58 pp. ISBN 951-666-227-7. ISSN 0781-2698.

Key words: Aluminum ores, aluminum chemicals, aqueous electrolytes, ionic activity

The activities of the hydrogen ion, the chloride ion, and the hypothetical H^+Cl^- species were determined in the system $HCl-AlCl_3-H_2O$ at ionic strengths $I = 1, 3, 5, 7$, and 10 mol/kg using the electromotive cell technique. Simultaneous measurement of the three emf's was possible using commercial $Ag,AgCl$ reference electrodes in a conventional Harned-type cell with Pt/H_2 and $Ag,AgCl$ electrodes as the primary electrodes.

Satisfactory agreement with the available mean activity data ($I = 1, 3$, and 5 mol/kg) was obtained. Single ion activities were compared with predicted data from the hydration theory and the Pitzer equations, the only available sources of reference. The disagreement between the experimental results and the predicted data were qualitatively interpreted in terms of hydration of the hydrogen ion and formation of $Al-Cl$ complexes.

It is believed that the experimental technique used will give better estimates of true single ion activities than the calculation methods until input parameters are known with better accuracy.

Heiskanen, T., *Application of Population Balances in Steady-State and Dynamic Studies of Two Particulate Processes: Crystallization and Emulsion Polymerization*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 171, Helsinki 1986, 23 pp. ISBN 951-666-228-5. ISSN 0781—2698.

Key words: Population balance, crystallization, emulsion polymerization.

Summary of a thesis which is a collection of five publications concerning application of population balances in crystallization and emulsion polymerization. The result of both of these processes is the formation of particles and their subsequent growth. The mathematical models of these two processes, and consequently the steady-state and dynamic behavior, are similar in many respects.

In the papers dealing with crystallization, steady-state and dynamic behavior of an MSMPR crystallizer with fines dissolving were studied, a stability criterion was derived, and crystallization of ammonium sulphate was simulated in numerical examples. The system was found to be stable under normal operating conditions.

In the papers dealing with emulsion polymerization, the mathematical model for continuous emulsion polymerization of vinyl chloride was developed and numerical examples of its steady-state solutions were given. Dynamics and stability of this system was studied using dynamic moment equations. The system was found to be stable or unstable depending on parameter values. In the cases studied the system was highly oscillatory. The dynamic responses were presented both in phase-space and time domain.

Palosaari, S.M., Parviaainen, S., Hiironen, J., Reunanen, J., and Neittaanmäki, P., *A Random Search Algorithm for Constrained Global Optimization*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 172, Helsinki 1986, 45 pp. ISBN 951-666-229-3. ISSN 0781—2698.

Key words: Nonlinear optimization, nonlinear simultaneous equations, random search optimization.

An new nonlinear optimization method is developed, based on alternating sequences of non-biased and concentrated random searches in the variable space. The reliability of the solution is essentially improved by comparing the results of independent iterations, and by accepting as a final result a variable vector which agrees with another result vector within the bounds of accuracy for each variable and which produces the best value of the objective function. The performance of the algorithm is tested with a number

of test functions, most of them of well-established use for testing purposes. Some of these functions derive from chemical engineering practice while some are purely mathematical by nature. It is shown that the method is reliable and that the consumption of computer time is within reasonable limits. It is also shown that the method can be successfully applied to the solution of small systems of nonlinear equations with constraints, by minimizing the sum of the squares of the implicit equations.

Ch 173

UDC 66.063

Laine, J., *Eine einfache halbgraphische Methode für die Formulierung der Funktion $Ne=f(Re)$ in der Rührtechnik aus einem bekannten Graph*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 173, Helsinki 1986, 24 pp. ISBN 951-666-233-1. ISSN 0781—2698.

Key words: Power-number, Reynolds-number, mixing.

This article (written in German) presents a simple semigraphic method to formulate the function $Ne=f(Re)$ with one or two hyperolas. With this equation it is possible to present the power of an impeller as a linear solution as soon as the rotation speed is chosen as a parameter in a given construction.

Ch 174

UDC 66.06

Niemi, H., Raimoaho, J., and Palosaari, S., *Modeling and Simulation of Ultrafiltration and Reverse Osmosis Processes*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 174, Helsinki 1986, 32 pp. ISBN 951-666-230-7. ISSN 0781—2698.

Key words: Ultrafiltration modeling, reverse osmosis modeling.

A model for membrane processes is developed to enable the calculation of permeate flux and rejection at different pressures and concentrations. The model is combined with a process simulation program which calculates all streams of the process.

The model is based on the finely porous model developed by Merten in which permeate flux and rejection are described with four quantities. The values of these quantities are constant for each system having the same solution, membrane and temperature. A method of obtaining the values of these quantities from experiments is described in the present work. The values were calculated from different amounts of experimental data to determine the minimum experimental information to enable the calculation of permeate flux and rejection over the entire operating range. The model was tested for ultrafiltration and reverse osmosis.

Ch 175

66.067:532.71

Laatikainen, M. and Lindström, M., *Separation of Methanol-Ethanol and Ethanol-n-Heptane Mixtures by Reverse Osmosis and Pervaporation*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 175, Helsinki 1986, 61 pp. ISBN 951-666-234-X. ISSN 0781—2698.

Key words: Liquid mixture separation, reverse osmosis, pervaporation.

The results obtained in the separation of binary methanol-ethanol and ethanol-n-heptane mixtures by reverse osmosis and pervaporation are presented. The fluxes and separation factors for homogenous cellulose acetate and poly(hexamethylene adipamide) membranes were measured at 298 K.

The experimental results were compared with values calculated from a membrane model based on the concepts of sorption equilibria and diffusive mass transport. The sorption interactions were interpreted with a modified Flory model and the transport equations were constructed by means of the friction coefficient formalism. The sorption parameters and diffusion coefficients of each binary and ternary system were determined experimentally.

In pervaporation, the calculated flux values coincide reasonably well with the experimental data in the whole composition range, but the separation factors can be predicted only approximately. The coupling effects observed in all systems were predominantly due to the swelling of the membranes. The correspondence of the theoretical and experimental values for reverse osmosis was less satisfactory.

Vuori, A., *Thermal and Catalytic Reactions of the C-O Bond in Lignin and Coal Related Aromatic Methyl Ethers*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 176, Helsinki 1986, 31 pp. ISBN 951-666-236-6. ISSN 0781-2698.

Key words: Carbon-oxygen bond, coal model compounds, hydrodeoxygenation, lignin model compounds, thermolysis

This paper summarizes the results of studies on thermolysis and catalytic hydrogenolysis of some simple lignin and coal related aromatic methyl ethers. The thermolysis of anisole as well as hydroxy and methoxy-anisoles follows the same reaction pattern. The main primary reaction pathways are the breaking of the methyl C-O bond, and the *ipso*-substitution of the methoxyl group. The breaking of the methyl C-O bond is the main primary reaction step also in the thermolysis of 4-propylguaiacol. The results are, however, insufficient for any hard conclusion about the significance of the *ipso*-substitution. Under hydrogen starvation conditions 4-propylguaiacol itself acts as a hydrogen donor.

The catalytic hydrogenolysis of 4-propylguaiacol on a CoMo hydrotreating catalyst leads to the breaking of the aromatic ring C-O bonds. This can be effected, to some extent, by the sulfur content of the catalyst which has also some effect on the selectivity of the formation of phenolic products. At the highest temperatures studied, complete deoxygenation of 4-propylguaiacol takes place and the products are also hydrogenated to some extent in the catalytic reaction.

Seppälä, J. and Ahvenainen, A. A., *Calculation of Process Variables in Slurry-Type Coordination Polymerization Reactors*. Acta Polytechnica Scandinavica, Chemical Technology and Metallurgy Series No. 177, Helsinki 1986, 34 pp. ISBN 951-666-238-2. ISSN 0781-2698.

Key words: Coordination polymerization, slurry polymerization

Polyethylene, polypropylene and heavier α -olefins can be polymerized with Ziegler-Natta catalysts in a slurry reactor. In this paper the variables affecting polymerization are discussed. Based on the simulation model designed, the effects of monomer concentration, residence time, catalyst activity, slurry concentration in reactor and catalyst deactivation rate were investigated.

It is necessary to optimize reactor conditions to achieve sufficient product purity and a high production rate at the same time. A relatively narrow operational window was shown to exist. Catalyst deactivation was shown to reduce the possibilities to reach low levels of catalyst residuals in the product.

CIVIL ENGINEERING AND BUILDING CONSTRUCTION SERIES

Ci 85

UDC 711.5(480):711.27

Teferra, A., *On the Issuing of Some Statements as a Part of Regional Physical Planning in Finland*. Acta Polytechnica Scandinavica, Civil Engineering and Building Construction Series No. 85, Helsinki 1986, 246 pp. + Appendix 289 pp. ISBN 951-666-237-4. ISSN 0355—2705.

Key words: Regional planning, evaluation, statements, Finland.

The position and significance of regional physical planning in Finland as a guideline to spatial development at the local level can be evaluated through an investigation and analysis of the relationships between the statements issued by the regional planning associations, the undertakings about which statements have been given, their location and the regional planning situation, the regional plans and objectives as well as the subsequent related decisions made by the authorities concerned. An overview of the regional physical planning system in Finland is given and a method for evaluating the guiding effects of regional planning on local planning and building developed by studying how the statements interpret and convey regional plans and objectives as well as the extent to which these have been considered in making decisions concerning planning and building at the local level. The research materials included a selection of the official statements of the Regional Planning Association of Satakunta addressed to 9 municipalities and to the Provincial Board between 28.11.1975 and 31.12.1982, the legal provisions and the state guidelines on the subject, the regional plans and objectives as well as the subsequent decisions. These have been inventoried, analyzed and compared with the help of tables, figures, etc. with respect to, a.o., statements as expressions of regional views and objectives, and measures and decisions taken by the authorities concerned. Comparisons of the regional views, the planning situation, the projects and the decisions at the above were used as a basis for the evaluation.

ELECTRICAL ENGINEERING SERIES

EI 56

UDC 621.38:616—073:539.143.43

Sepponen, R.E., *Discrimination and Characterization of Biological Tissues with Magnetic Resonance Imaging: A Study on Methods for T1, T2, T1g and Chemical Shift Imaging*. Acta Polytechnica Scandinavica, Electrical Engineering Series No. 56, Helsinki 1986, 44 pp. ISBN 951-666-226-9. ISSN 0001—6845.

Key words: Nuclear magnetic resonance, magnetic resonance imaging.

The paper summarizes six publications constituting the thesis for the degree of Doctor of Technology. The papers of this work consist of studies and developments of methods for discrimination and characterization of biological tissues with T1, T2, T1g and chemical shift magnetic resonance imaging. Special consideration has been given to the detection and characterization of intracranial hematomas. Clinical studies have been done utilizing two different strengths of the polarizing magnetic field. At 0.17 T a characteristic visualization of chronic subdural hematomas has been demonstrated with T1 and T2 weighted imaging. The differentiation of an acute intracranial hematoma has been shown to be superior at 0.02 T compared to 0.17 T. A characteristic visualization of the lesion has been demonstrated by suitable T1 and T2 weighted imaging sequences at 0.02 T. A new chemical shift imaging method has been described. A visualization of a human pathology with the proton chemical shift imaging at 0.17 T has been reported. A method for T1g imaging has been described and a visualization of a human pathology has been reported.

Ph 154

UDC 531.44:685.363.522

Erkkilä, J., Pihkala, P., Rahikainen, A., and Spring, E., *Studies of the Mechanical Properties of Cross-Country Skis*. Acta Polytechnica Scandinavica, Applied Physics Series No. 154, Helsinki 1986, 24 pp. ISBN 951-666-232-3. ISSN 0355-2721.

Key words: Ski, snow, mechanics, friction.

A device for measuring the effect of a force acting on a ski has been constructed. The device can also be used for simulating the backward push of a skier on the ski. The force distribution of the sole of the ski on the underneath layer, i.e. the snow surface, has been measured for different cross-country skis. Of these skis 6 were classified as functioning satisfactorily and 4 unsatisfactorily according to the opinion of experienced skiers. The well-functioning skis were observed to have a more symmetric force distribution against the snow surface than the poor ones. Moreover, the modulus of elasticity, the vibration including its damping, and the efficiency (i.e. the energy consumed in damping divided by the energy consumed in bending the ski during one swing) were measured and studied. Clear differences were found in the efficiency of the skis between the well and bad functioning skis. The place of binding was found to effect the backward push of the ski, but not its gliding properties.

Ph 155

UDC 535.33:621.315.59:539.23

Lahtinen, J.A., *Electro-Optical Studies of Semiconductor Compounds for Electroluminescent and Laser Devices*. Acta Polytechnica Scandinavica, Applied Physics Series No. 155, Helsinki 1986. 51 pp. ISBN 951-666-239-0. ISSN 0355-2721.

Key words: Electroreflectance, ZnS, electroluminescent display. InP, InGaAsP, fiber communication laser.

Summary of a thesis, which consists of six publications discussing properties of the semiconductor compounds used in high field electroluminescence display devices and optical fiber communication lasers. Some interesting critical points, in particular the absorption edge, of ZnS, InP and InGaAsP as a function of growth conditions, doping and composition, respectively, are studied by means of the electroreflectance technique. It is shown that the growth temperature, reactant materials and growth method each has a contribution to the crystalline properties of the zinc sulfide thin films. An accurate method is developed to determine the energy gaps from the overlapping electroreflectance line profiles. Using this new method, the band population effects in indium phosphide are studied, and the composition dependence of four energy gaps in InGaAsP is described. The electrical and optical properties of novel InGaAsP/InP laser structures are characterized with emphasis on their performance in variable temperature and modulation conditions. Modifications in the construction of the double channel planar buried heterostructure laser result in improvements on temperature susceptibility. The V-groove distributed feedback laser is proved to be a remarkable dynamic single mode device.

MATHEMATICS AND COMPUTER SCIENCE SERIES

Ma 46

UDC 681.518.52

Visuri, P., *Intelligent Multivariate Process Supervision*. Acta Polytechnica Scandinavica, Mathematics and Computer Science Series No. 46, Helsinki 1986, 79 pp. ISBN 951-666-231-5. ISSN 0355—2713.

Key words: Process supervision, alarm systems, artificial intelligence, man-machine systems.

This thesis addresses the difficulties encountered in managing large amounts of data in supervisory control of complex systems. Some previous alarm and disturbance analysis concepts are reviewed and a method for improving the supervision of complex systems is presented. The method, called multivariate supervision, is based on adding low level intelligence to the process control system. By using several measured variables linked together by means of deductive logic, the system can take into account the overall state of the supervised system. Thus, it can present to the operators fewer messages with higher information content than the conventional control systems which are based on independent processing of each variable. In addition, the multivariate method contains a special information presentation concept for improving the man-machine interface.

APPLIED PHYSICS SERIES

Ph 153

UDC 550.837.32:519.64

Eloranta, E.H., *Studies on Integral-Equation Based Modeling of Mise-à-la-Masse Anomalies for Geophysical Surveying*. Acta Polytechnica Scandinavica, Applied Physics Series No. 153, Helsinki 1986, 42 pp. ISBN 951-666-225-0. ISSN 0355—2721.

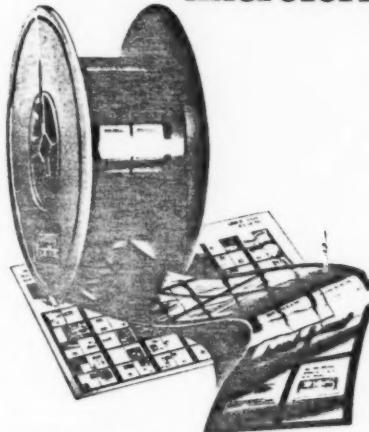
Key words: Mise-à-la-masse method, electrical methods, numerical modeling, integral equation technique, galvanic anomalies.

This paper summarizes four papers that deal with the modeling of mise-à-la-masse anomalies by means of integral equation methods and the characteristics of these anomalies. Two different formulations are applied: 1) Fredholm's integral equation of the 1st kind, based on the equipotential state of the conductors solved together with the supplementary equations derived from the equation of continuity, and 2) the case of a finite conductivity contrast (the ratio of the conductivity of the body to that of the environment) formulated by means of Fredholm's integral equation of the 2nd kind for the potential. The development of the equipotential state as a function of the conductivity contrast is examined with the aid of the latter equation. The integral equations are solved numerically by the method of subareas. Two different configurations of the subarea division are examined, and the results obtained compared. In the first configuration the subareas are as long as the model along the strike, and the end faces of the model are omitted. In the second configuration the whole boundary of the model is divided into subareas. At the end of the paper a few practical problems raised in exploration surveys and solved by means of the modeling methods developed are presented.

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ACTA POLYTECHNICA SCANDINAVICA**... a Scandinavian contribution to international engineering sciences**

1958-1971 published under the auspices of the Scandinavian Council for Applied Research

in *Denmark* by the Danish Academy of Technical Sciencesin *Finland* by the Finnish Academy of Technology, the Swedish Academy of Engineering Sciences in Finland and the State Institute for Technical Researchin *Norway* by the Norwegian Academy of Technical Sciencein *Sweden* by the Royal Swedish Academy of Engineering Sciences

As of 1972 the journal is published by the Finnish Academy of Technology. The Editor-in-Chief is Professor Mauri Luukkala and the editorial secretary is Ari Rautsara.

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